NRC·CNRC

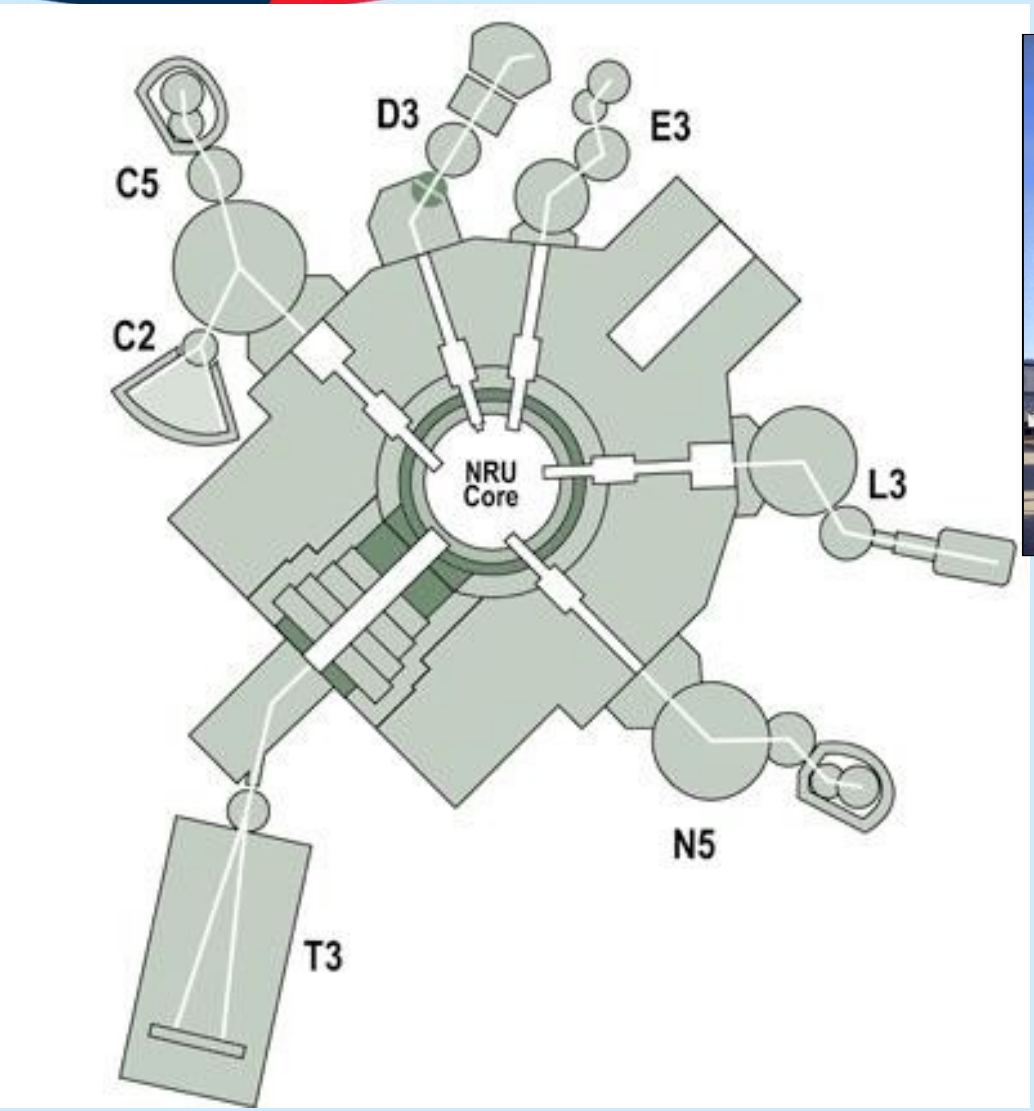
From Discovery to Innovation…

Supporting Scientists' at NRC-CNBC

Mark Vigder

Canadian Neutron Beam Centre

Canadian Neutron Beam Centre (CNBC)



- 24/7 operation
- 5 beams for R&D on ‘hard materials’
- 1 beam for R&D on thin films
- 1 beam for R&D on soft materials (under development)

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My background
(and prejudices)

- Background in software engineering
  - practitioner and researcher
- Employed by the National Research Council Canada
  - NRC conducts research on different scientific and engineering topics (medical instruments, building construction, iceberg towing, neutron scattering,...)
- Work with scientists on how they use software and how they develop software
  - Ocean technology, aerospace, …
- Relative newcomer to neutron scattering
  - currently updating the data acquisition and control system at the CNBC

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My past life:

A simple system for scientific workflows

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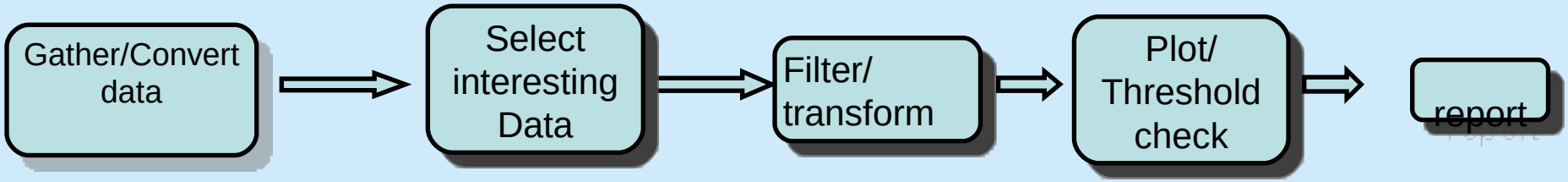
Scientific workflows



- A sequence of steps, performed during an experiment, to transform, manage, analyze and display data
  - Same steps performed many times for each experiment
- Issues:
  - sequence done manually or represented by short programs
  - Steps are similar each time they are executed, but with slight variations
  - Programs are copied modified
  - Various sw tools used, COTS, legacy, …

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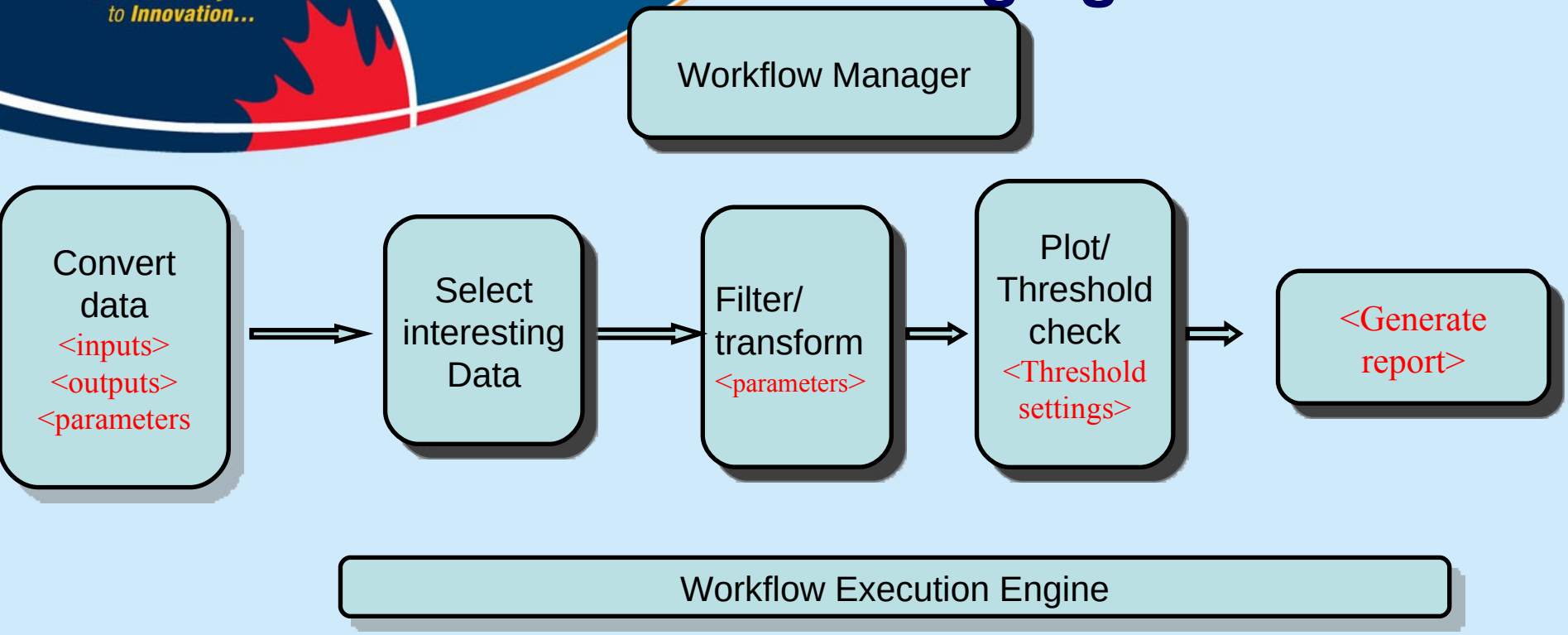
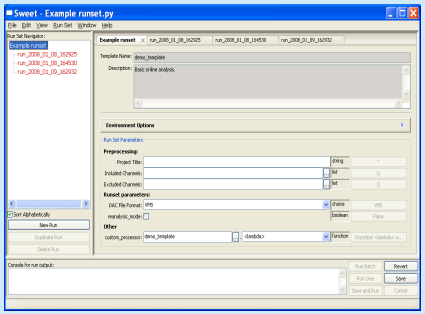
Managing workflows



Each step in workflow is parameterized tool invocation

Workflow manager:

- Locates available workflows
- Lists recently executed workflows
- Dynamically creates GUI for workflow invocation
- Name and descriptions for workflow invocations (runs)



Workflow Execution Engine:

- Location of workflow template with parameters

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Results

- Easily automatable operations are easy to automate
  - Sometimes even by the scientists
- Many programming operations or now done at the GUI level
  - GUI is automatically generated
- Minimize ‘cloning and modifying’
  - Single version of the program. Only parameters at invocation are different.
  - Simplifies versioning
- Easier to automate tedious workflows
  - Standard tool integration mechanisms
  - Integration of off-the-shelf tools into workflows

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My future life:

Bring the computer systems for CNBC up to modern standards

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CNBC Current System: the good

- Highly reliable
- Very functional
  - Developed by beamline scientists to meet very specific needs
- Adaptable in many dimensions
  - Customizing interface, describing experiment configuration,...
- Remote access
  - For many years!
- SIMPLE!! In two important ways
  - Simple to use
  - Software design is simple

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CNBC Current System: the bad

- Software and hardware technology are obsolete
- It's adaptability has hit the wall
- Cannot take advantage of new technologies
- Stand alone system, difficult to integrate
  - Not required to integrate with other systems and it meets that requirement 100%

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CNBC System requirements

- Functional requirements are easy
  - Do what the current system does
- The major constraint: PEOPLE
  - Entire lab is about 25 people
  - There will never be more than 2 or 3 people devoted to software development and maintenance
- Software lifecycle:
  - 30 years+ (control and data acquisition system)
  - Data reduction/analysis easier to change (5 - 15 years)
- Integrating off-the-shelf (OTS) tools for much of the functionality
  - See lack of PEOPLE
  - Let the beamline scientists do what they are already doing
    - Extensive use made of Excel for scan definition, data analysis.

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IPython shell

Command line based:
- -GUI takes too much time
- -Easier to get api right
- -Add GUI later
- -See lack of PEOPLE

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IPython shell

Python:
-Simple – relatively easy to learn,
-'batteries included'
-Fully functional language
-Good support, particularly in scientific community
-Easy to wrap other off-the-shelf sw tools

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IPython shell

IPython:
-I'm not writing my own shell
-Configurable, extensible, embeddable
-Integrated with numPy, SciPy, matplotlib

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IPython shell

Epics Channel Access Tools

EPICS IOC

EPICS:
-Is there any reason not to use EPICS?
-No programming (just a hell of a lot of configuration)

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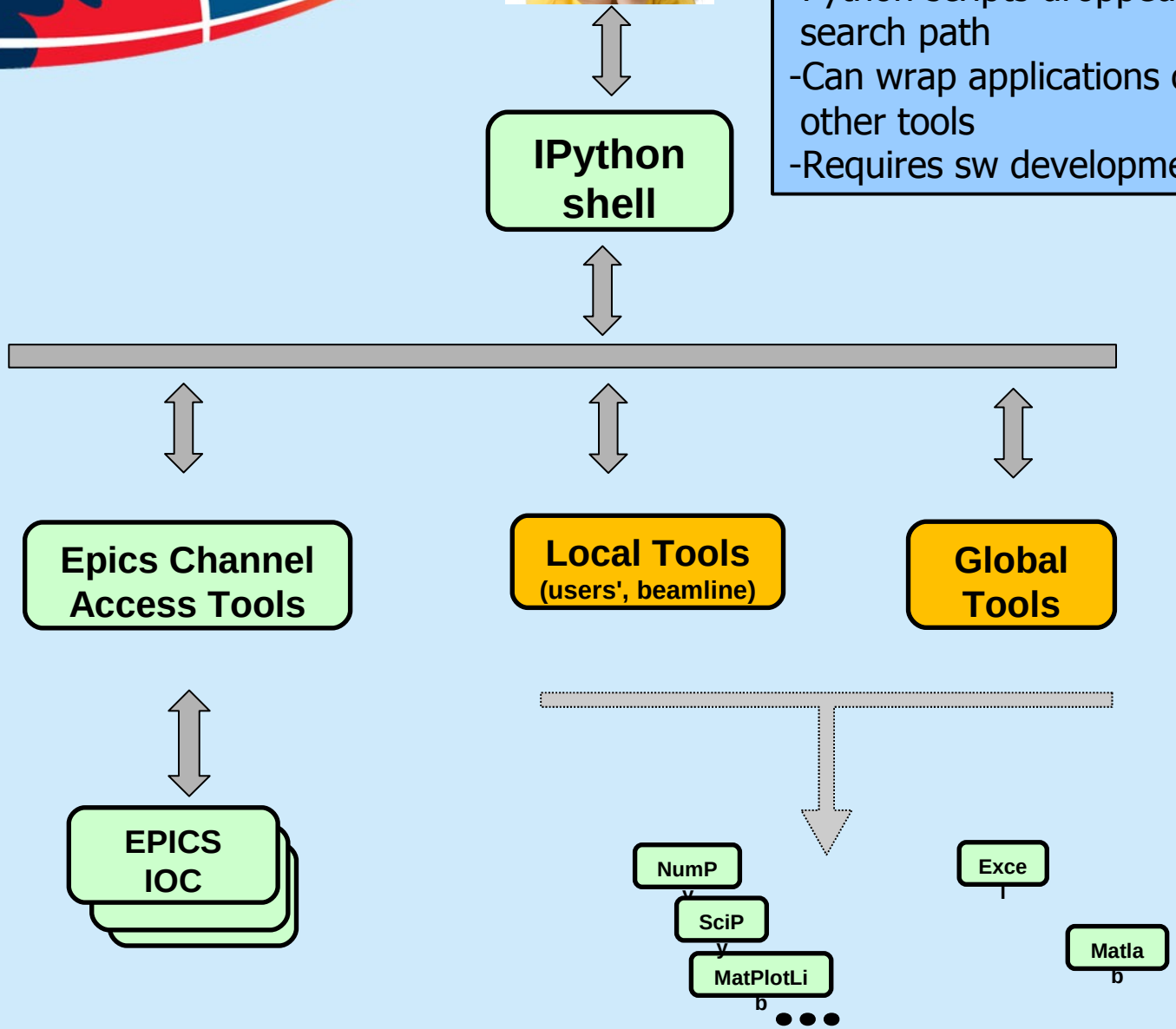
Tools:
- Python scripts dropped on the search path
- Can wrap applications or use other tools
- Requires sw development



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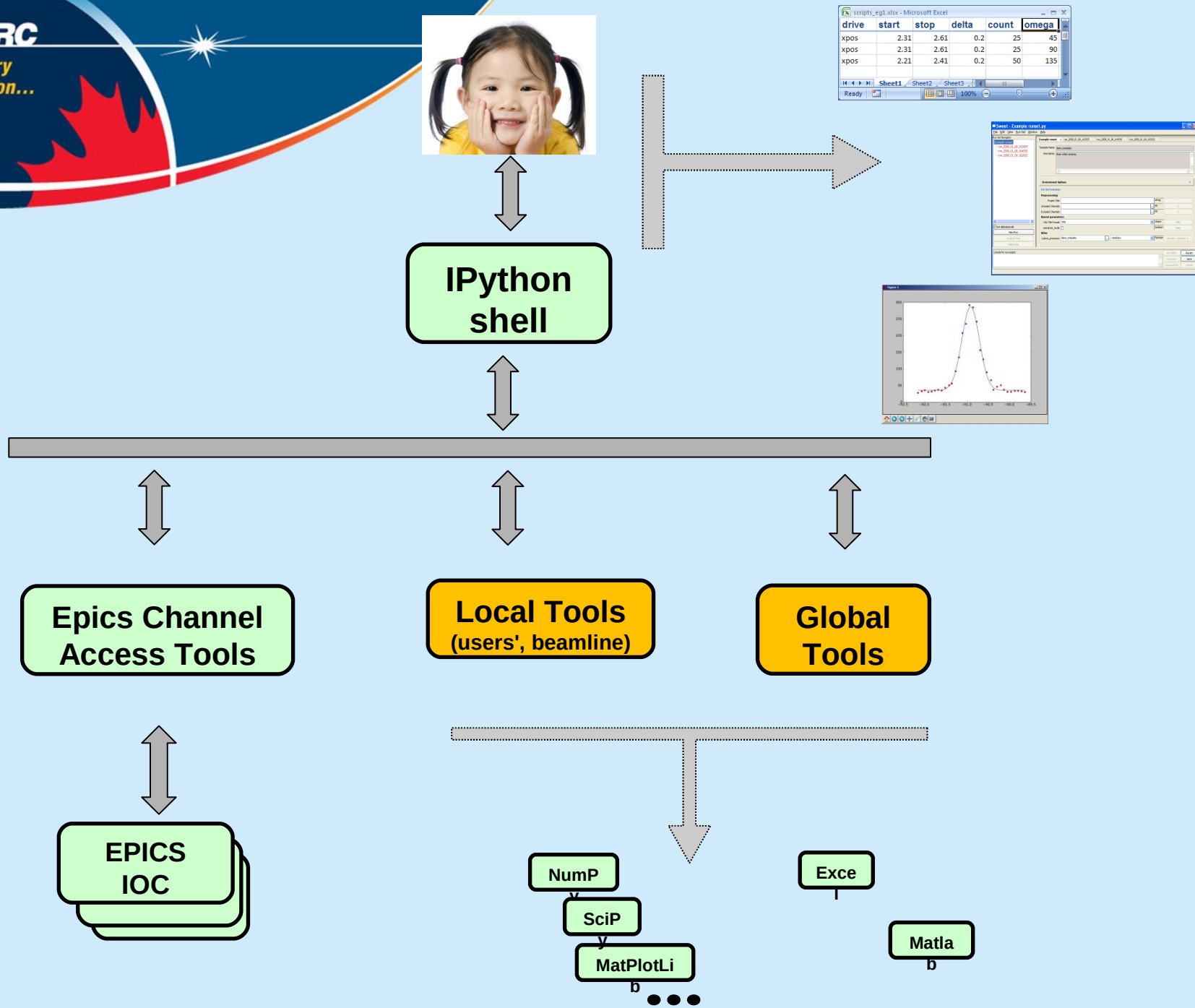

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Questions